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PI Index of Zig-Zag Polyhex Nanotubes

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Abstract

The Padmakar–Ivan (PI) index of a graph G is defined as PI(G) = $\sum[n_{eu}(e|G)+ n_{ev}(e|G)]$, where $n_{eu}(e|G)$ is the number of edges of G lying closer to u than to v, $n_{ev}(e|G)$ is the number of edges of G lying closer to v than to u and summation goes over all edges of G. The PI Index is a Szeged-like topological index developed very recently. In this paper an exact expression for PI index of the zig-zag polyhex nanotubes is given.

1. Introduction

Graph theory was successfully provided the chemist with a variety of very useful tools, namely, the topological index. A topological index is a numeric quantity from the structural graph of a molecule.

The Wiener index (W) is the oldest topological indices. Numerous of its chemical applications were reported and its mathematical properties are well understood [1-5]. We encourage the reader to consult [6], for a good survey on the topic.

In Refs. [7,8], the authors defined a new topological index and named it Padmakar-Ivan index. They abbreviated this new topological index as PI. This newly proposed topological index, PI, does not coincide with the Wiener index (W) for acyclic

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(trees) molecules. The derived PI index is very simple to calculate and has a discriminating power similar to that of the W index, for details see [9-11].

We now recall some algebraic definitions that will be used in the paper. Let G be a simple molecular graph without directed and multiple edges and without loops, the vertex and edge-shapes of which are represented by V(G) and E(G), respectively. If e is an edge of G, connecting the vertices u and v then we write e=uv. The number of vertices of G is denoted by n. The distance between a pair of vertices u and w of G is denoted by $d_G(u,w)$. We define for e=uv two quantities $n_{eu}(e|G)$ and $n_{ev}(e|G)$. $n_{eu}(e|G)$ is the number of edges lying closer to the vertex u than the vertex v, and $n_{ev}(e|G)$ is the number of edges lying closer to the vertex v than the vertex u. Then the Padmakar–Ivan (PI) index of a graph G is defined as $PI(G) = \sum[n_{eu}(e|G)+ n_{ev}(e|G)]$. We notice that the edges equidistant from both ends of the edge uv are not counted in calculating the PI index of a graph. In fact, if $G_{u,e} = \{x \mid d_G(u,x) < d_G(v,x)\}$, $G_{v,e} = \{ x \mid d_G(u,x) > d_G(v,x)\}$ and $G_e = \{x \mid d_{G-\{e\}}(u,x) - d_{G-\{e\}}(v,x) = \pm1\}$ then $n_{eu}(e|G) = |E(G_{u,e})|$, $n_{ev}(e|G) = |E(G_{v,e})|$ and $N(e) = |E(G_e)|$. Here for any subset U of the vertex set V = V(G), |E(U)| denotes the number of edges of G between the vertices of U. It is easy to see that $|E(G)| = N(e) + n_{eu}(e|G) + n_{ev}(e|G)$.

In a series of papers, Diudea and coauthors [12-18] computed the Wiener index of some nanotubes. In this paper an exact expression for PI index of zig-zag polyhex nanotubes is given. Our notation is standard and mainly taken from [12-14] and [19,20]. Throughout this paper $T = TUHC_6[2p,q]$ denotes an arbitrary zig-zag polyhex nanotube, in the terms of their circumference (2p) and their length (q)**.**see Figure 1.

2. PI Index of $TUHC_6[2p,q]$

In this section, the PI index of the graph $T = TUHC_6[2p,q]$ were computed. To do this, we assume that E = E(T) is the set of all edges of T and $N(e) = |E| - (n_{eu}(e|G) + n_{ev}(e|G))$. Then $PI(T) = |E|^2 - \sum_{e\in E} N(e)$. But $|E(T)| = p(3q-1)$ and so $PI(T) = p^2(3q-1)^2 - \sum_{e\in E} N(e)$. Therefore, for computing the PI index of T, it is enough to calculate N(e), for every $e \in E$. To calculate N(e), we consider two cases that e is horizontal or non-horizontal.

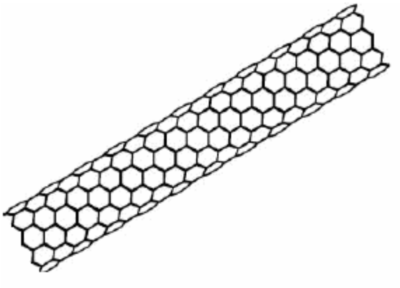

Figure 1: Zig-zag $TUHC_6[20,q]$ (The figure is taken from [17])

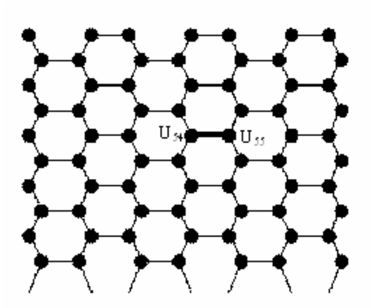

Figure 2: A Zig-Zag Polyhex Lattice with p=5 and q=7

Lemma 1. *If e is an horizontal edge then N(e) = p.*

Proof. Suppose $e = U_{ij}U_{i(j+1)}$ denotes an arbitrary horizontal edge of i^{th} row of the zig-zag polyhex lattice of $TUHC_6[2p,q]$, Figure 2. It is obvious that for every k, $0 \le k \le p-1$, $U_{(i+2k)j}U_{(i+2k)(j+1)}$ is an horizontal edge parallel to e and $d_T(U_{ij},U_{(i+2k)j}) = d_T(U_{i(j+1)},U_{(i+2k)(j+1)}) = 2k$. Thus $\{U_{ij},U_{(i+2)j}, \ldots, U_{(i+2p-2)j},U_{i(j+1)},\ldots,U_{(i+2p-2)(j+1)}\} \subseteq T_e$. We now prove the equality of two sets. To do this, we assume that $U_{kl}U_{(k+1)l}$ is an arbitrary non-horizontal edge of T. If $l \le j$ then $d_T(U_{kl},U_{ij}) < d_T(U_{kl},U_{(i+1)j})$ and $d_T(U_{(k+1)l},U_{ij}) < d_T(U_{(k+1)l},U_{(i+1)j})$ and so $U_{kl} \notin T_e$. In other case $U_{(k+1)l} \notin T_e$. A similar argument shows that every horizontal edge of T_e must be parallel to e. Thus $\{U_{ij},U_{(i+2)j}, \ldots, U_{(i+2p-2)j},U_{i(j+1)},\ldots,U_{(i+2p-2)(j+1)}\} = T_e$. Therefore, N(e) = p, proving the lemma. □

Lemma 2. *If e is a non-horizontal edge in the k^{th} column, $1\le k \le p$, of the* zig-zag polyhex lattice of $T = TUHC_6[2p,q]$, *then* $N(e) = \begin{cases} 2p+2(k-1) & q \ge p+k-1 \\ 2q & q \le p+k-1 \end{cases}$.

Proof. Let E_{ij} denote the non-horizontal edge of T in the i^{th} row and j^{th} column. We first notice that for every j, $1\le j \le q$, $N(E_{1j}) = N(E_{2j}) = \cdots = N(E_{(2p)j})$. So it is enough to calculate $N(E_{11}), N(E_{12}), \cdots, N(E_{1q})$. Compute the value of $N(E_{11})$. Suppose $q \ge p$. We consider the edges $E_{(p+1)1}$, $E_{(p+1)2}$, ⋯, $E_{(p+1)p}$. If $1 \le t \le p$ then $E_{(p+1)t} = U_{(p+1)t}U_{(p+2)t}$ and we have $d_T(U_{(p+1)t},U_{21}) = d_T(U_{(p+2)t},U_{11}) = p+t-2$. So $E_{(p+1)t} \in E(T_{E_{11}})$, $1 \le t \le p$. Similarly, for $0 \le i \le p-2$, $E_{(2p-i)(i+2)} \in E(T_{E_{11}})$ and $E(T_{E_{11}}) \subseteq \{E_{(p+1)1}, E_{(p+1)2}, \cdots, E_{(p+1)p}, E_{11}, E_{(2p)2}, \cdots, E_{(p+2)p}\}$. To prove the equality, we assume that $U_{kl}U_{(k+1)l}$ is an arbitrary non-horizontal edge of T. If $l \ge p+1$ then $d_T(U_{kl},U_{21}) < d_T(U_{kl},U_{11})$ and $d_T(U_{(k+1)l},U_{21}) < d_T(U_{(k+1)l},U_{11})$ and so $U_{kl}U_{(k+1)l} \notin E(T_{E_{11}})$. If $l \le p$ then we have exactly two edges in every column belong to $\{E_{(p+1)1}, E_{(p+1)2}, \cdots, E_{(p+1)p}, E_{11}, E_{(2p)2}, \cdots, E_{(p+2)p}\}$ and other edges of this column don't belong to $E(T_{E_{11}})$. Therefore $E(T_{E_{11}}) = \{E_{(p+1)1}, E_{(p+1)2}, \cdots, E_{(p+1)p}, E_{11}, E_{(2p)2}, \cdots, E_{(p+2)p}\}$. If $q \le p$ by above calculations $E(T_{E_{11}}) = \{E_{(p+1)1}, E_{(p+1)2}, \cdots, E_{(p+1)q}, E_{11}, E_{(2p)2}, \cdots, E_{(2p+2-q)q}\}$. We continue our argument by considering the edge E_{12}. To prove this case, we delete the first column of the zig-zag polyhex lattice and obtain a $TUHC_6[2p,q-1]$. Since E_{12} is the (1,1) entry of this lattice, we have

$$N(E_{12}) = R + \begin{cases} 2p & q-1 \ge p \\ 2q-2 & q-1 \le p \end{cases},$$

where R is the number of edges $E(T_{E_{12}})$ in the first column of $TUHC_6[2p,q]$. On the other hand, $E_{(p+1)1}$ and $E_{(2p)1}$ are only edges of $TUHC_6[2p,q]$ in the first column. Therefore,

$$N(E_{12}) = \begin{cases} 2p+2 & q \ge p+1 \\ 2q & q \le p+1 \end{cases}.$$

We can continue this method for computing $N(E_{13})$, ⋯, $N(E_{1p})$ to complete the proof. □

Lemma 3. *If $q \le 2p$ then* $N(E_{11}) = N(E_{1q})$, $N(E_{12}) = N(E_{1(q-1)})$, ⋯, $N(E_{1s}) = N(E_{1(s+1+b)})$, where $s = [q/2]$, the greatest integer less than or equal to q/2, and $b = [(q+1)/2] - [q/2]$.

Proof. Since the zig-zag polyhex lattice is symmetric, the proof is straightforward. □

Lemma 4. *If $q > 2p$ then $N(E_{11}) = N(E_{1q})$, $N(E_{12}) = N(E_{1(q-1)})$, ⋯, $N(E_{1p}) = N(E_{1(q-p+1)})$, and $N(E_{1(p+1)}) = N(E_{1(p+2)}) = \cdots = N(E_{1(q-p)}) = N(E_{1p})$.*

Proof. The first part of the lemma is a conclusion of this fact that the zig-zag polyhex lattice is symmetric. To prove the second part, we notice that for a fixed column j there are exactly 2p-1 columns with two edges belongs to $E(T_{E_{1j}})$. The other columns don't intersect $E(T_{E_{1j}})$. Thus $N(E_{1(p+1)}) = N(E_{1(p+2)}) = \cdots = N(E_{1(q-p)}) = N(E_{1p})$. □

We now ready to state the main result of the paper. We have:

Theorem. The PI index of the zig-zag polyhex nanotube is as follows:

$$PI(TUHC_6[2p,q]) = \begin{cases} p^2(9q^2-7q+2)-4pq^2 & if \quad q \le p \\ p^2(9q^2-15q+4p-2)+4pq & if \quad q \ge p \end{cases}.$$

Proof. Since $PI(T) = |E|^2 - \sum_{e\in E} N(e)$, it is enough to compute $\sum_{e\in E} N(e)$. Suppose X and Y are the set of all horizontal and non-horizontal edges of T. Then

$$PI(T) = |E|^2 - \sum_{e\in X} N(e) - \sum_{e\in Y} N(e)$$

$$= p^2(9q^2-7q+2) - \begin{cases} 4p\sum_{i=1}^{p} N(E_{1i}) + 2p(q-2p)N(E_{1p}) & if \quad q \ge 2p \\ 4p\sum_{i=1}^{q-p+1} N(E_{1i}) + 2p(2p-q-2)N(E_{1(q-p+1)}) & if \quad p < q < 2p \\ 2pqN(E_{11}) & if \quad q \le p \end{cases}.$$

By Lemma 2, $N(E_{1i}) = N(E_{11}) + 2(i-1)$ and so we have:

$$PI(T) = p^2(9q^2-7q+2) - \begin{cases} 2pqN(E_{11}) + 4p(p-1)(q-p) & if \quad q \ge 2p \\ 2pqN(E_{11}) + 4p(p-1)(q-p) & if \quad p < q < 2p \\ 2pqN(E_{11}) & if \quad q \le p \end{cases}$$

$$= p^2(9q^2-7q+2) - \begin{cases} 4pq^2 & if \quad q \le p \\ 4p(2pq-p^2-q+p) & if \quad q \ge p \end{cases},$$

which completes the proof. □

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